ABSTRACT

A set of spectral data is collected from a mixture and corrected to remove instrumental artifacts. The collected mixture spectra define an n-dimensional data space, where n is the number of data points in the spectra. Principal component analysis (PCA) techniques are applied to the n-dimensional data space to generate and select a subset of m eigenvectors that effectively describe all variance in the original data space. The members of a spectral library of known, pure components are examined based on this reduced dimensionality data space using target factor testing techniques. Each library spectrum is represented as a vector in the m-dimensional reduced data space, and target factor testing results in an angle between the library vector and the data space for each spectral library member. Those spectral library members that have the smallest angles with the data space are considered to be potential members, or candidates, of the mixture and are submitted for further testing. The spectral library members are ranked and every combination of the top y members is considered as a potential solution to the composition of the mixture. A multivariate least-squares solution is then calculated using the mixture spectra for each of the candidate combinations. Finally, a ranking algorithm is applied to each combination and is used to select the combination that is most likely the set of pure components in the mixture.

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